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SUMULATION METHOD
[SHIMYURE-SHON HOHO]

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(54) [Title of the Invention]

SIMULATION METHOD

[Claim(s)]

[Claim 1] A method for simulating the diffusion of an impurity or point defects in a semiconductor manufacturing process; said simulation method characterized by setting a boundary condition in the boundary of a region where simulation is performed so that the impurity or point defects are allowed to move across the boundary of a calculation region.

[Claim 2] The simulation method of Claim 1 characterized by determining the boundary condition of the applicable boundary so that the amount of movement of the impurity or point defects going across the applicable boundary is equalized to the amount of movement obtained when the aforesaid amount of movement is calculated in a sufficiently wide region including the applicable region for the aforesaid boundary condition.

[Claim 3] The simulation method of Claim 1 characterized by determining the boundary condition, whereby the impurity moves past the boundary by using the fine coefficient of the impurity profile in the normal direction of the boundary near the boundary for the aforesaid boundary condition.

[Claim 4] The simulation method of Claim 1 characterized by determining the boundary condition for the aforesaid boundary condition, whereby the impurity or point defects move past the boundary by approximating the impurity or point defects profile using a Gauss function in the normal direction of the boundary near the boundary for the aforesaid boundary condition.

[Detailed Specifications]

[0001] [Technical Field of the Invention]

The present invention relates to a simulation method, and in particular, a technique used in simulating the diffusion of an impurity or point defects in a semiconductor manufacturing process.

[0002] [Prior Art]

Owing to higher integrated circuits, the number of manufacturing steps has increased and the steps themselves have become complicated. Thus, the number of trials has increased and development costs have risen. To deal with such circumstances, great efforts have been exerted to narrow the trial conditions, curtail the number of trials, and shorten the trial period by using a simulation. For example, in the case of a process simulation, the processing conditions of the trial were narrowed so that ion implantation, oxidation and diffusion steps, and the like were simulated using a process simulation, and the shape of the elements and the impurity distributions were measured, with desired results.

[0003] A process simulation has problems if simulation is done in a wide element region because the calculations take time. An impurity diffusion simulation occupies the majority of the calculation time and memory capacity required for the process simulation. Therefore, if the calculation time and memory capacity required for an impurity diffusion simulation in a wide region is curtailed, the process simulation can be performed with good efficiency.

[0004] To perform a high-speed impurity diffusion simulation with a small memory capacity, the simulation region must be limited to the

necessary part(s). However, because a reflection-type boundary condition has been used in a conventional impurity diffusion simulation, there were problems because the impurities became trapped in the boundary when the calculation region was narrow, and the solving accuracy decreased. In order to simplify this, an example of a one-dimensional simulation of a step for forming a well will be described.

[0005] Figure 3 is a graph when boron was ion-implanted in a silicon substrate at 100 keV and a dose of $3\times10^{13}/cm^2$. The X axis of this chart is the depth from the surface of the silicon substrate and the Y axis is the boron concentration. The dotted line **A** in the graph represents the profile immediately after ion implantation. Moreover, the results obtained by calculating a boron profile when boron has diffused for 4 hours at 1,200°C, from the surface of the substrate to a depth of 8 μm in order for an accurate calculation, is shown by the dashed line **B**.

[0006] Generally, since there should be a profile of many of the element characteristics to calculate the threshold of, e.g., a MOSFET where the depth from the surface of the substrate is 2 μm, the calculation is often performed by limiting the calculation region to this region for reasons such as to shorten the processing time. The profile in this case is shown by the dot-and-dash line **C**. In either case, a reflection-type boundary condition is made use of at the bottom of the substrate. By narrowing the calculation region from this graph, the solving accuracy becomes extremely poor, as seen from the result shown by the dot-and-dash line **C**.

[0007] [Problems to be Solved by the Invention]

When a reflection-type boundary condition was used for the boundary of the impurity diffusion simulation region in this way, there was a problem because the solving accuracy diminished when the calculation region was narrowed. Meanwhile, when the simulation region was widened for performing an accurate simulation, the memory capacity thus required was increased and there was a problem because the calculation time was prolonged.

[0008] The present invention was achieved in view of the above-mentioned circumstances and it is an object to provide a simulation method capable of obtaining a highly accurate solution in a narrow calculation region.

[0009] [Means for Solving the Problems]

In order to accomplish the above-mentioned object, the invention of Claim 1 is a method for simulating the diffusion of an impurity or point defects in a semiconductor manufacturing process, which is characterized by setting a boundary condition in the boundary of a region where simulation is performed so that the impurity or point defects are allowed to move across the boundary of a calculation region.

[0010] The invention of Claim 2 is characterized by determining the boundary condition of the applicable boundary so that the amount of movement of the impurity or point defects going across the applicable boundary is equalized to the amount of movement obtained when the amount of movement is calculated in a sufficiently wide region including the applicable region for the boundary condition in Claim 1.

[0011] The invention of Claim 3 is characterized by determining the boundary condition, whereby the impurity moves past the boundary by using

the fine coefficient of the impurity profile in the normal direction of the boundary near the boundary for the boundary condition of Claim 1

[0012] The invention of Claim 4 is characterized by determining the boundary condition for the boundary condition in Claim 4, whereby the impurity or point defects move past the boundary by approximating the impurity or point defects profile using a Gauss function in the normal direction of the boundary near the boundary for the aforesaid boundary condition.

[0013] [Embodiments of the Invention]

The embodiments of the simulation method pertaining to the present invention will now be described in reference to the drawings. To simplify the description in the embodiments below, a 1-dimensional impurity diffusion simulation for a silicon substrate is carried out.

[0014] In the simulation method described according to the embodiments below, an ordinary computer system is used which is provided with a CPU for performing various processings, input devices, such as a keyboard, mouse, light pen and flexible disk device, external storage devices, such as a memory device and disk device, output devices, such as a display device and printer, etc. Moreover, the aforesaid CPU is equipped with, among other units, an arithmetic logical unit which performs the processing or the like in each step described below, and a main memory part in which the instructions for the aforesaid processings are stored.

[0015] 1^{st} embodiment

Figure 1 is a flowchart showing the processing operation for an impurity diffusion simulation of this embodiment. When the diffusion simulation

is started, the diffusion time **T** is set to 0 (Step S101). The diffusion equation is set (Step S102) by calculating the diffusion coefficient, segregation coefficient, and the like at the diffusion temperature.

[0016] The boundary of the simulation region, that is, the boundary condition for the substrate bottom in this example is set, as mentioned below (Step S103).

[0017] $F = -D \cdot \partial C / \partial x$

Here, **D** is the impurity diffusion coefficient and **C** is the impurity concentration. This boundary condition means that the impurity has spilled out of the simulation region through the bottom of the substrate according owing to the flux **F**. The reflection-type condition in the conventional method was set as the boundary condition here. Thus, the impurity distribution that should be spread by the diffusion is the reflection-type boundary condition set at the bottom, so the impurity becomes trapped and its concentration is significantly increased. This problem could have been avoided by setting the simulation region sufficiently wide, but then that presented a problem because the calculation time was prolonged.

[0018] The solution of the diffusion equation is obtained using a numerical analysis while setting the diffusion equation and the boundary condition (Step S104). Next, the diffusion time **T** is increased by **ΔT** (Step S105), and whether or not the value thereof exceeds a total diffusion time **Tf** is judged (Step S106). If it does not, the loop is executed again after setting the diffusion equation in Step S102, and if it is, the calculation ends.

[0019] The advantages of the present invention are described next in an example of a one-dimensional diffusion simulation of boron in a silicon substrate. Figure 2 is a graph when the boron is ion-implanted in the silicon substrate at 100 keV and a dose of $3\times10^{13}/cm^2$. The X axis of this chart is the depth from the surface of the silicon substrate and the Y axis is the boron concentration. To simplify the description, calculations were made as if there was no evaporation of the impurity from the substrate surface. Here, the result obtained by doing an accurate calculation by diffusing the boron for 4 hours at 1,200°C, with the depth of the substrate sufficient at 8 μm, is shown by the dashed line **B**. Moreover, the dot-and-dash line **C** is a result obtained by limiting the depth of the substrate to 2 μm and performing the calculation using the conventional method, in which a reflection-type boundary condition is used as the boundary condition for the substrate bottom. Therefore, the boron becomes trapped in the calculation region and the boron concentration is overestimated. Meanwhile, the result obtained by limiting the depth of the substrate to 2 μm in the calculation using the present invention is shown by the solid line.

[0020] The result according to the simulation method pertaining to the present invention is shown by the thick line **D**. This result matches extremely well a result (dashed line **B**) calculated accurately because of the sufficiently wide region since the boundary condition of the simulation boundary, as illustrated, is provided suitably, even though the simulation boundary is limited to 2 μm. The impurity distribution close to the substrate surface is affected significantly by the element characteristics. As

shown in Fig. 2, in the present invention, the impurity distribution close to the substrate surface is accurately calculated; hence, the elemental characteristics can be obtained highly accurately.

[0021] By using the present invention in this way, a simulation can be performed without losing any accuracy at all even if the simulation region is narrowed. In this example, the simulation region is curtailed by one-fourth, but it goes without saying that the memory capacity and calculation time required for the simulation can be curtailed to the same degree. A high-speed process simulation can be performed using a smaller memory capacity than in the past by using the present invention.

[0022] Moreover, a simplified description in this embodiment was thus performed using a one-dimensional simulation, but it is obvious that the present invention can be applied to a 2- or 3-dimensional simulation. In particular, it is seen that the effects of curtailing the memory capacity and calculation time is remarkable in a 2- or 3-dimensional simulation.

[0023] 2nd embodiment

Whereas the boundary condition was calculated in the 1st embodiment using the differential of the impurity distribution in setting the boundary condition in Step S103, the boundary condition should be set so that a solution close to the solution calculated in a wider region is obtained. Therefore, in this embodiment, the profile in the normal direction of the boundary of the impurity distribution near the boundary is approximated according to a Gauss function:

$a \cdot \exp[-b(x-x_0)^2]$

in the case of a one-dimensional simulation.

Here, **x** represents the depth from the substrate surface and **a**, **b** and $\mathbf{x_0}$ are constants. As is well known, the Gauss function is the solution of the diffusion equation when the diffusion coefficient is a constant. As a consequence, the impurity distribution near the bottom of the simulation region can be approximated accurately by a Gauss function. The flux at the boundary is calculated as this Gauss function exceeds the simulation boundary and extends outside the boundary, and its value is used as the boundary condition. Since a numerical differential, such as in the above-mentioned embodiment, is not used when the boundary condition is calculated in the above process, a stable calculation is enabled without depending on a mesh interval, etc. As a result, a simulation result can be obtained more accurately than in a conventional method.

[0024] 3rd embodiment

Diffusion of an impurity in a silicon substrate was described in the above embodiments, but diffusion of an impurity can be applied to a point defects and impurity diffusion simulation. Since an impurity diffusion affects the point defects, this impurity diffusion can be described more accurately by a diffusion equation incorporating defect points than a diffusion equation using just an impurity.

[0025] However, since the diffusion rate of the point defects was markedly faster than that of an impurity, it was necessary to significantly widen the simulation region when a conventional method was used. For example, the calculation region in the process simulation for a MOSFET usually is about 10 μm deep from the surface of the substrate, but approximately several 100 μm is required if the point defects are incorporated.

Thus, because a large amount of memory was needed for a simulation incorporating a point defects diffusion, the calculation time was significantly prolonged.

[0026] However, a calculation region required for diffusion of just an impurity is set, for example, and in the 1st embodiment the boundary condition is applied to point defects in a method used for an impurity. A simulation is enabled even in a region as narrow as when just an impurity diffusion is handled, and the required memory capacity and calculation time can be curtailed drastically.

[0027] As described above, by using these embodiments of the simulation method, a process simulation for a semiconductor element can be performed just the necessary region. Therefore, it is possible to perform a high-speed simulation with a smaller memory capacity than in the past. Moreover, although, in the conventional method, the accuracy of the obtained calculated result may be extremely poor if the simulation region is narrowed, by using the present invention, a reduction in the calculation accuracy is suppressed even if the simulation region is narrowed; hence, the possibility of being perplexed by a result calculated with poor accuracy can be reduced.

[0028] As described in the 1st embodiment, if the boundary condition is calculated using the differential of an impurity profile in the normal direction of the boundary, the advantages of the present invention can be realized by fine-tuning conventional programs. Moreover, the calculation time required for calculating the boundary condition is substantially so negligibly short as compared to the calculation time required for a simulation.

[0029] Moreover, as described in the 2nd embodiment, the boundary condition is assumed if the profile is approximated by a Gauss function in the normal direction of the boundary of the impurity distribution near the boundary and this function is extended outside the boundary, the flux is calculated at the boundary by calculating the flux at the boundary and using it. Since the boundary condition can be set with such an arrangement without using a numerical calculation, a boundary condition independent a mesh or the like used in a numerical calculation can be set.

[0030] Furthermore, as described in the 3rd embodiment, the boundary condition can be applied to not only an impurity diffusion, but also to a point defects and impurity diffusion simulation. Since the diffusion rate of an impurity was markedly high for point defects, it was necessary to significantly widen the simulation region when a conventional method was used. Thus, a large amount of memory was required for a simulation incorporating point defects diffusion, and the calculation time was prolonged significantly. However, by applying the present invention, a simulation is enabled even in a narrow region and the required memory capacity and calculation time can be curtailed drastically.

[0031] Moreover, programs for realizing the aforementioned simulation method can be stored on a recording medium, which is read by a computer system. As a result, the aforementioned simulation method can be realized while controlling the computer by executing the aforesaid programs. Here, the aforesaid recording medium may comprise a device, such as a memory device, magnetic disk device or optical disk device able to record programs.

[0032] [Advantages of the Invention]

As described above, according to the simulation method pertaining to the present invention, a highly accurate solution can be obtained even in a narrow calculation region while performing the simulation of the diffusion of an impurity, point defects, and the like in a semiconductor manufacturing process.

[Brief Description of the Drawings]

[Figure 1] is a flowchart depicting a processing in an embodiment of the simulation method pertaining to the present invention.

[Figure 2] is a graph depicting a well impurity distribution when a process simulation is performed according to the simulation method of this embodiment. The X axis is the depth from the substrate surface and the Y axis is the boron concentration.

[Figure 3] is a graph depicting the impurity concentration of a well when a conventional process simulation method is used. The X axis shows the depth from the substrate surface and the Y axis shows the boron concentration.

[Explanation of the Codes]

A: boron concentration distribution immediately after ion implantation thereof

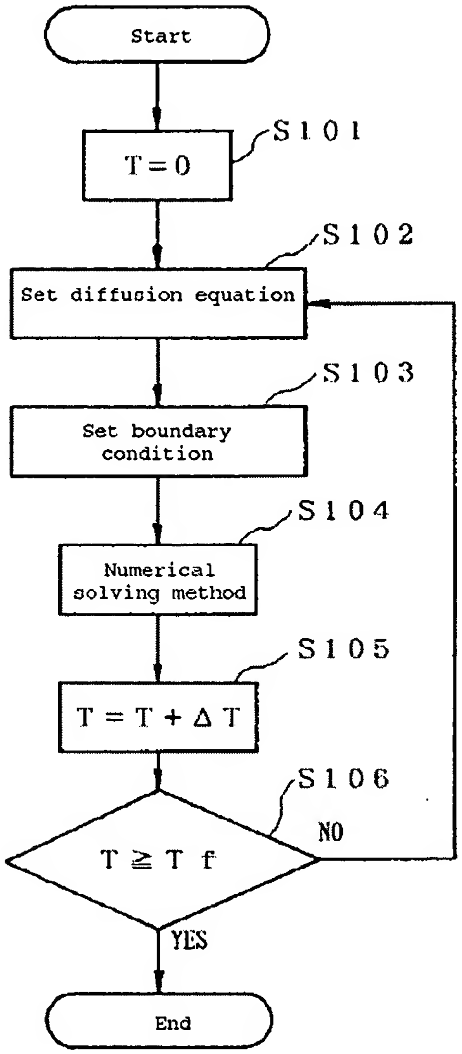
B: boron concentration distribution curing calculation to depth of 8 μm

C: boron concentration distribution during calculation to depth of 2 μm

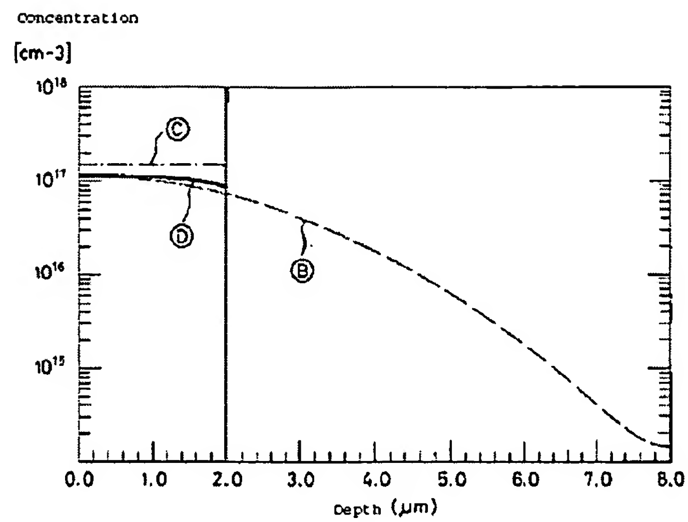
D: boron concentration distribution during calculation to a depth of

2 μm using the simulation method of this embodiment

[Figure 1]



[Figure 2]



[Figure 3]